2-D data reduction using Nika package, part II

Reducing data with Nika

This handout describes how to reduce 2D SAXS (pinhole) data using Nika package. In this case we use data collected on 15ID beamline during February 2010. Note, that the data reduction varies from instrument to instrument, this is just one of methods how to reduce the data.

This handout has number of parts. This is part II – data reduction itself. This handout assumes you have Igor experiment from Part I.

Experiment description (aka: what you need to know):

We used MarCCD detector. This is detector, which produces, in 2x2 binning, 1k x 1k images (with circular active area, see below). The pixel size is (after 2x2 binning) 0.158mm x 0.158mm. Image file format is Tiff.

We used 12keV X-ray radiation (1.0332 A).

Our detector was approximately 570mm from the sample area.

We collected following frames to provide calibration and data corrections:

Dark image at necessary times

Empty beam shot at necessary times

Ag Behenate measurement (distance/beam center calibration)

Glassy Carbon measurement (intensity calibration). Note: transmission of Glassy Carbon is: 0.818 at this energy.

We measured transmissions for samples, provided below:

Sa1 was measured as 0.943

Sa2 was measured as 0.979

Sa3 was measured as 0.960

Sa4 was measured as 0.968

Note, that in part I of this handout we optimized the data and also calculated Calibration constant for this setup to be (for 5 second measurement) 0. 0008445. For other times needs to be scaled by 5/exposure time.

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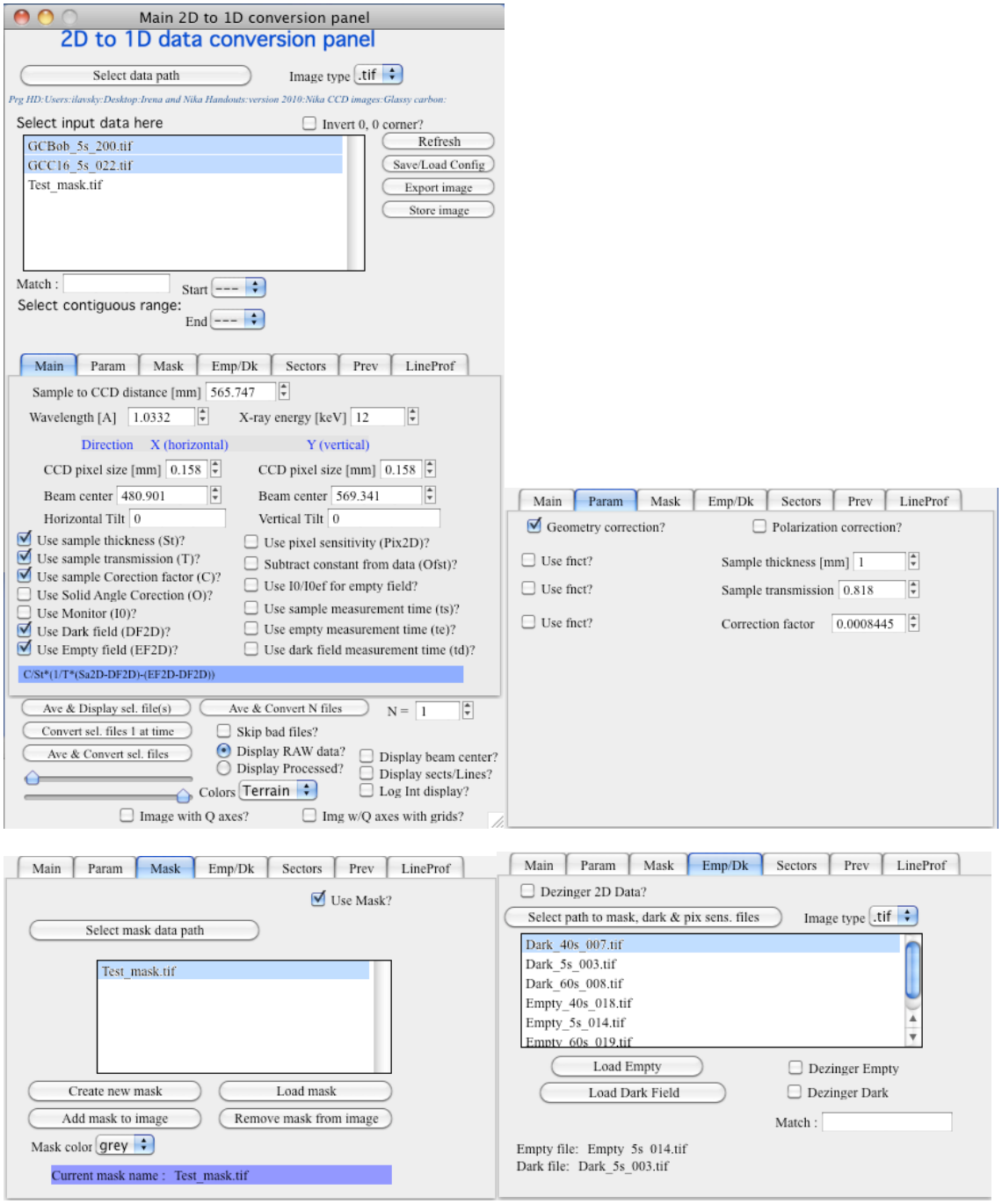
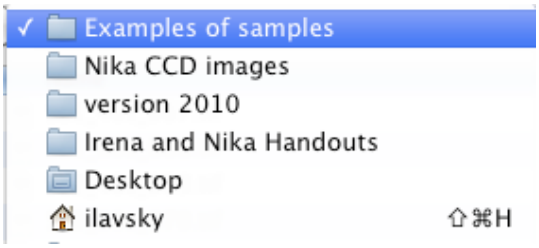
Resulting Nika setup from Part I



Sample data reduction

Now we need to find the right samples, scale the scaling constant for exposure time and find the right empty and dark… So lets start.

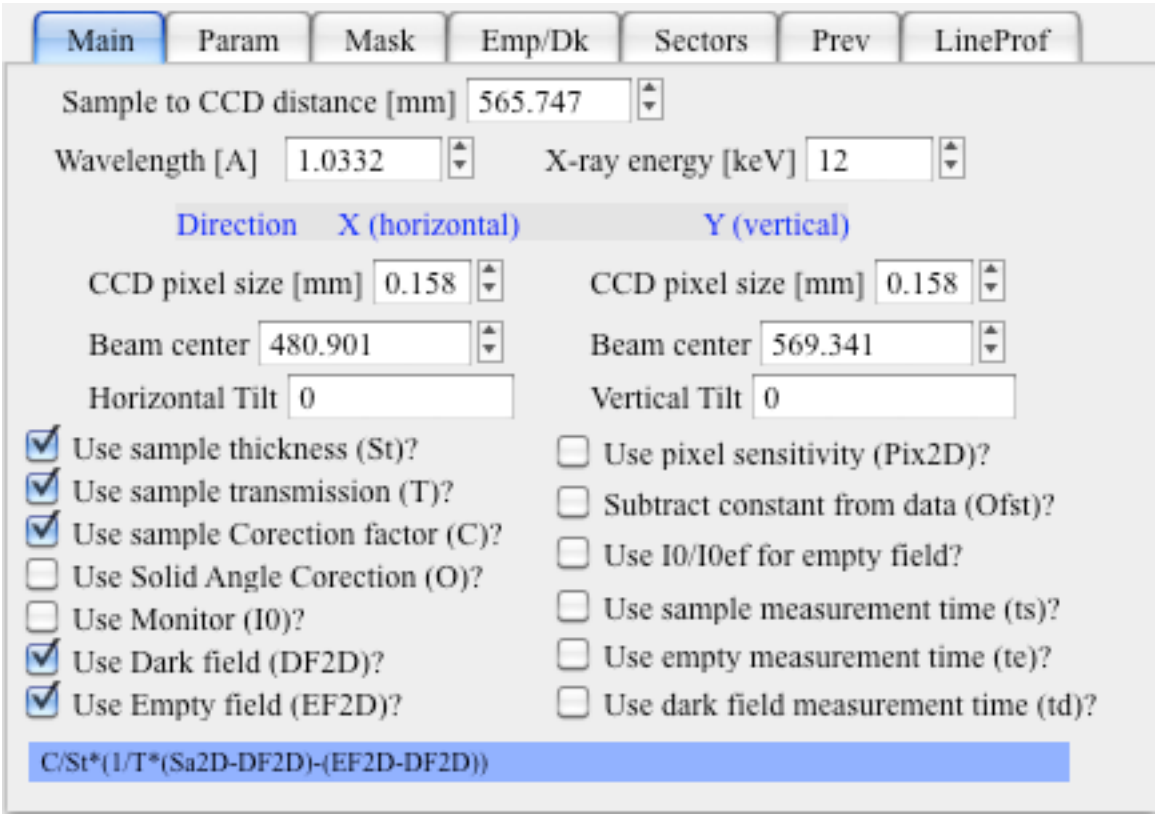
First use button “Select Data path” at the top of the Main panel to select path to experimental data:



Note, we have images collected for 40 seconds or 60 seconds. Let’s analyze only the 40-second measurements. In this case you can use “Match” filed below the list box and input in it *40s* . Now only files containing 40s will be listed.

Next we need to setup the parameters as appropriate.

The “Main” tab:



The “Params” tab will contain thickness – assume these samples were about 0.3 mm each. We need transmissions:

Sa1 was measured as 0.943

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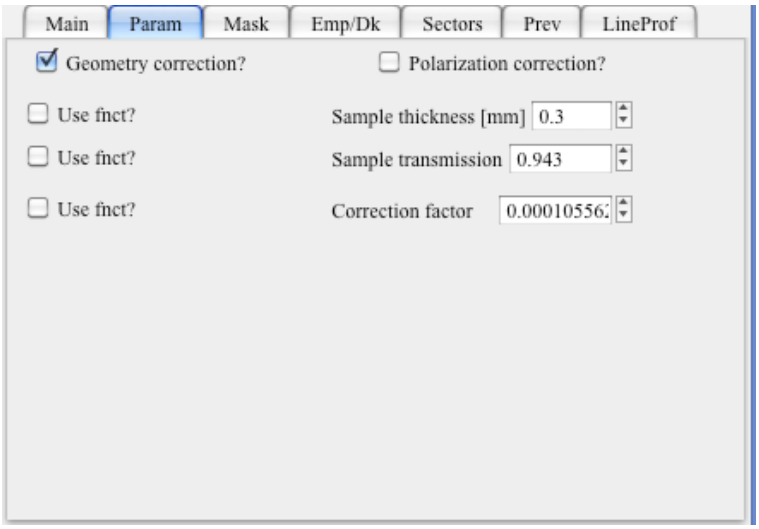
Sa2 was measured as 0.979

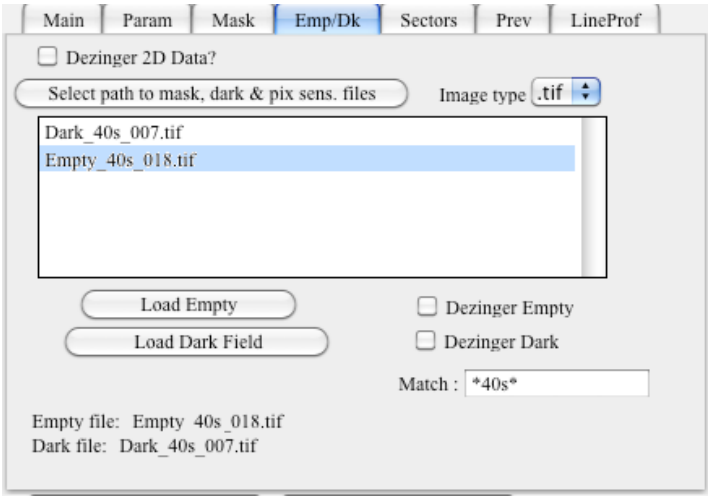
Sa3 was measured as 0.960

Sa4 was measured as 0.968

And calibration constant for 40 seconds is 0.000105562 (0.0008445 * 5 / 40). Here is the tab for Sa1:



Mask tab is the same, Emp/Dk tab we need to replace the Empty and Dark with 40 seconds measurements. Select the right file and load them in using the buttons:



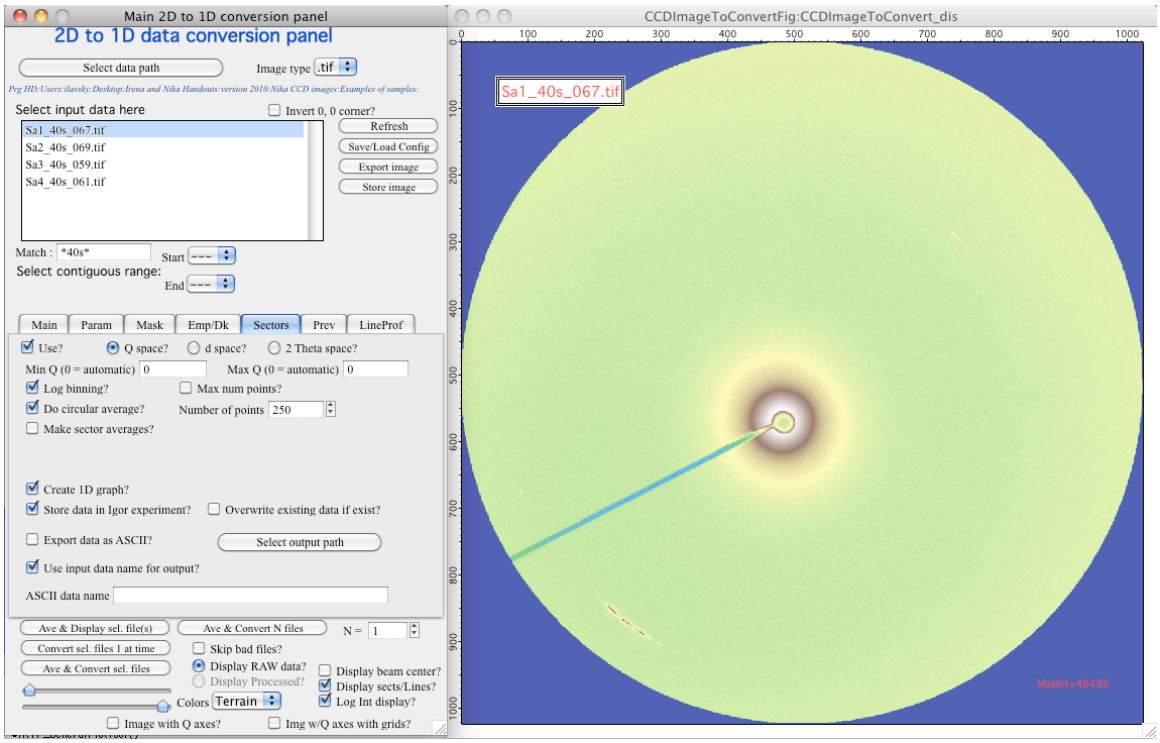
Now Nika should be setup to reduce data for sample 1.

Sectors analysis

Using the tools in the "Sectors" tab is the fastest and most convenient way of reducing data in transmission geometry when you have large number of data

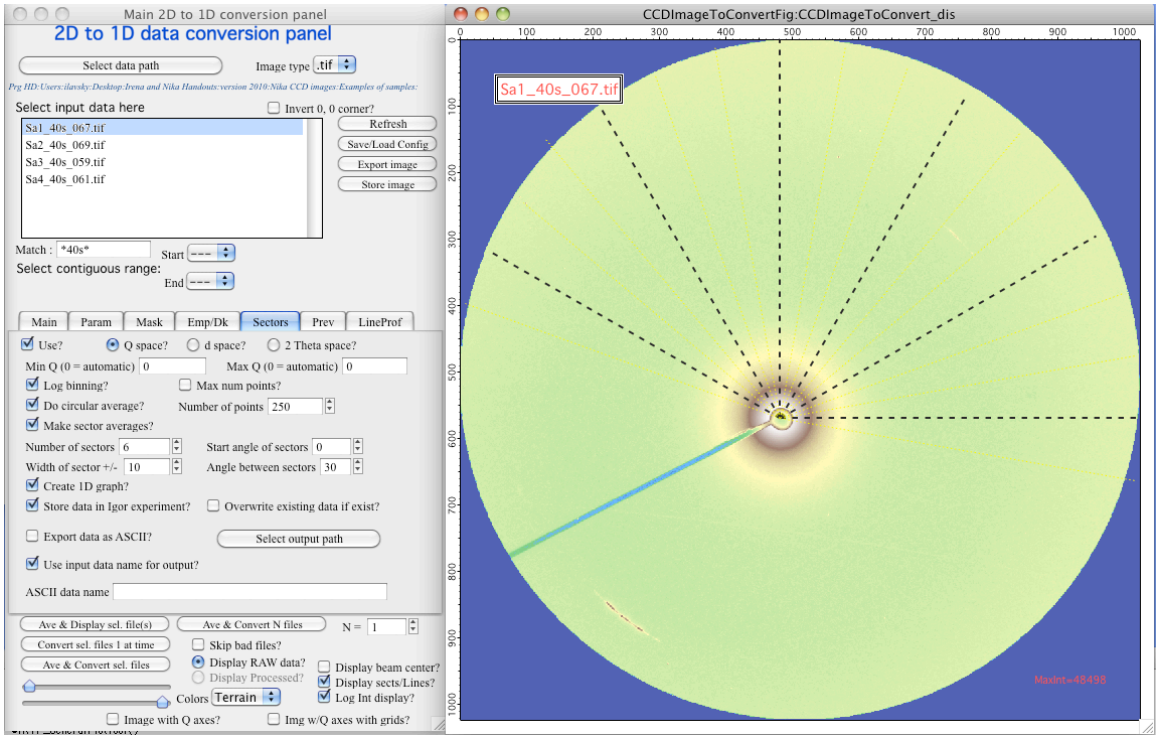
images collected in the same conditions. This tab enables to reduce data either in circular average or in various sectors. This enables users to reduce data of isotropic samples (using Circular average) or anisotropic samples (where these sectors are appropriate). Let's setup some analysis :

First we need to have an image to see changes on, so select the "Sa1_40s…tif" and push button "Ave & Display sel. File(s)". Also choose few checkboxes at the bottom right corner of the Main Panel: "Display sects/Lines" and "Log Int. display".



At this moment we have only Circular average checked, so there is not much displayed in the image.

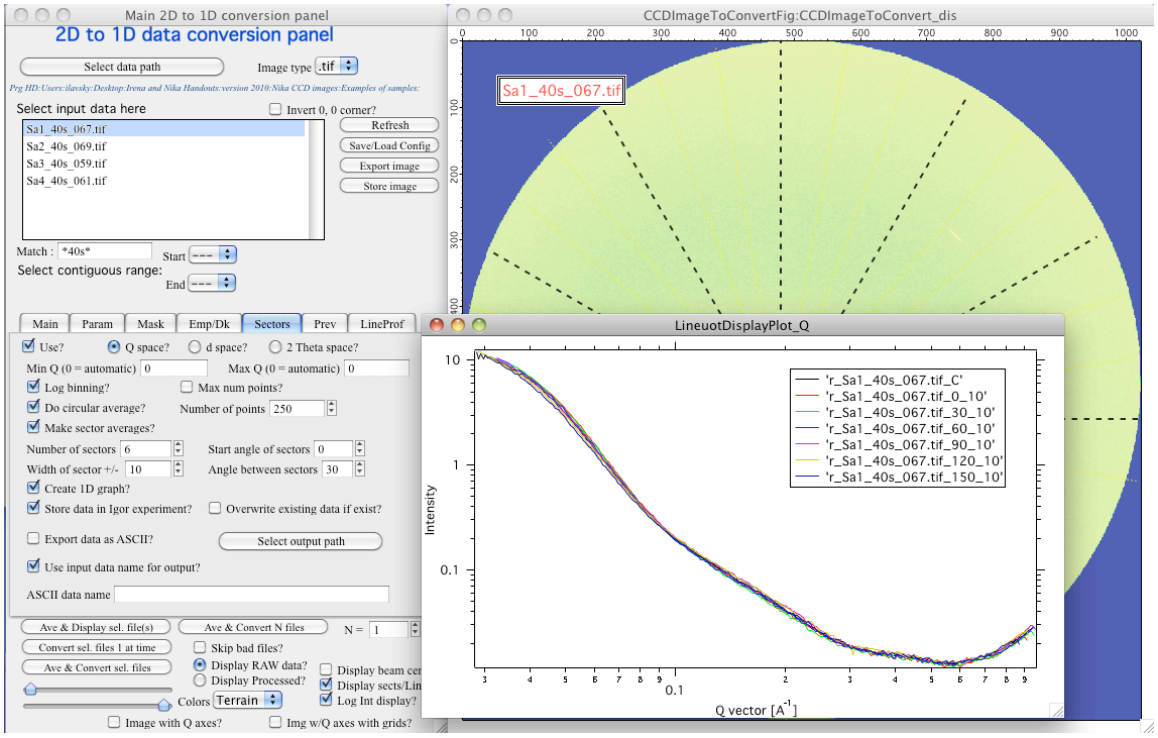
Now, check "Make sector averages?" also and put number of sectors to 6, leave Start angle at 0, width to +/- 10 and change Angle between sectors to 30:



The black lines are sector center lines, the Yellow lines indicate edges of the sectors – for each sector Nika will integrate between the two yeallo lines and present the data as if they were along the black central line.

Depending on anisotropy (and yes, this is isotropic figure, so it is not much help) the width of sector may need to be increased or reduced. Too narrow sectors produice very noisy data.

Now select “Convert sel. Files 1 at time” and see what happens:



We have got results with :

1. Circular average, note Nika used (as chosen) file name for sample name and added _C at the end.

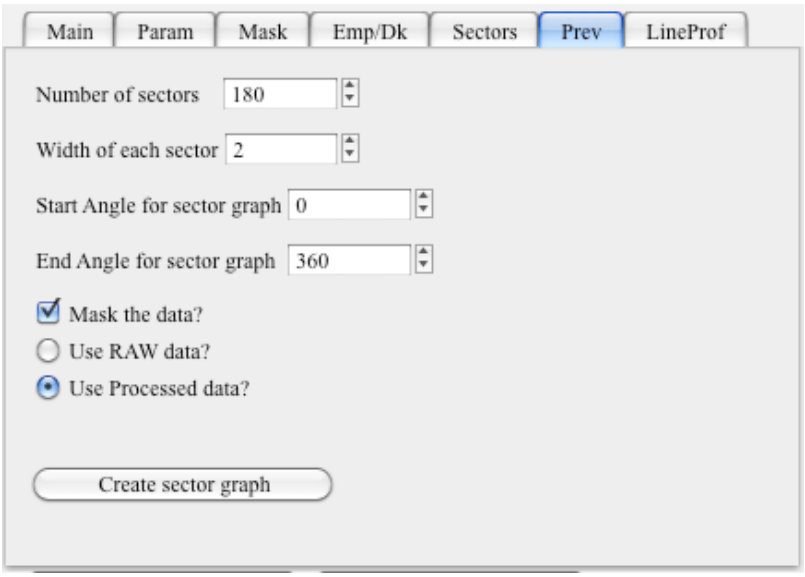
2. 6 secotr averages (all same results, it is isotropic sample), again sample anme is the image name,but added at the end is _XX_YY, where XX is Angle of the center line and YY is the half-width of the sector.

So this is one of the methods to reduce data. To reduce the other data sets, select other data set, correct manually the transmission and push button “Convert sel. Files 1 at time”.

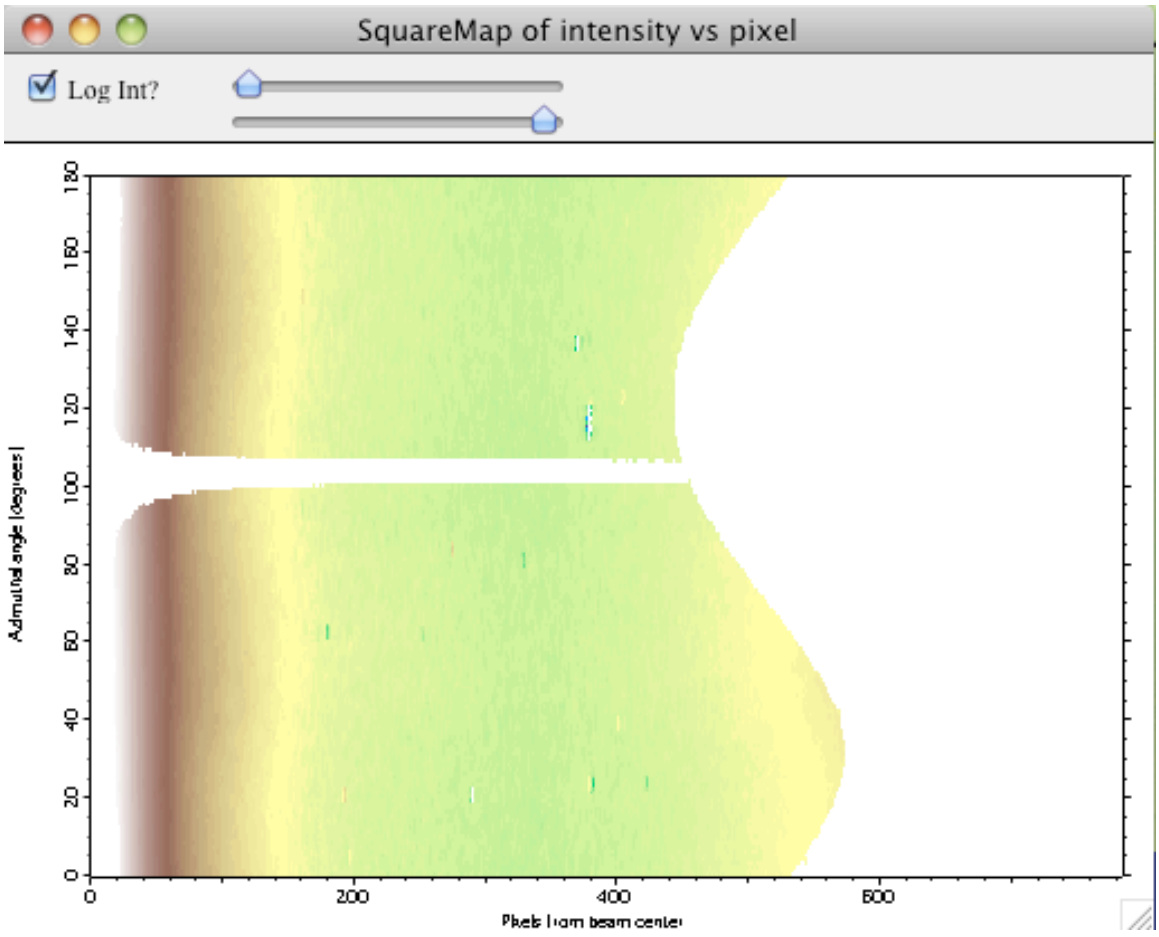
Prev

This is “preview” type screen. It helps one to play with the data to see, what is happening. Following will try to explain partially, what can be done. First, uncheck the checkbox “Use” on the “Sectors” tab and select the “Prev” tab. checkbox.

Reduce the Number of sectors to 180 (this will reduce the Width to 2), select “Mask the data?” and leave rest as it is:



Push button “Create sector graph”:



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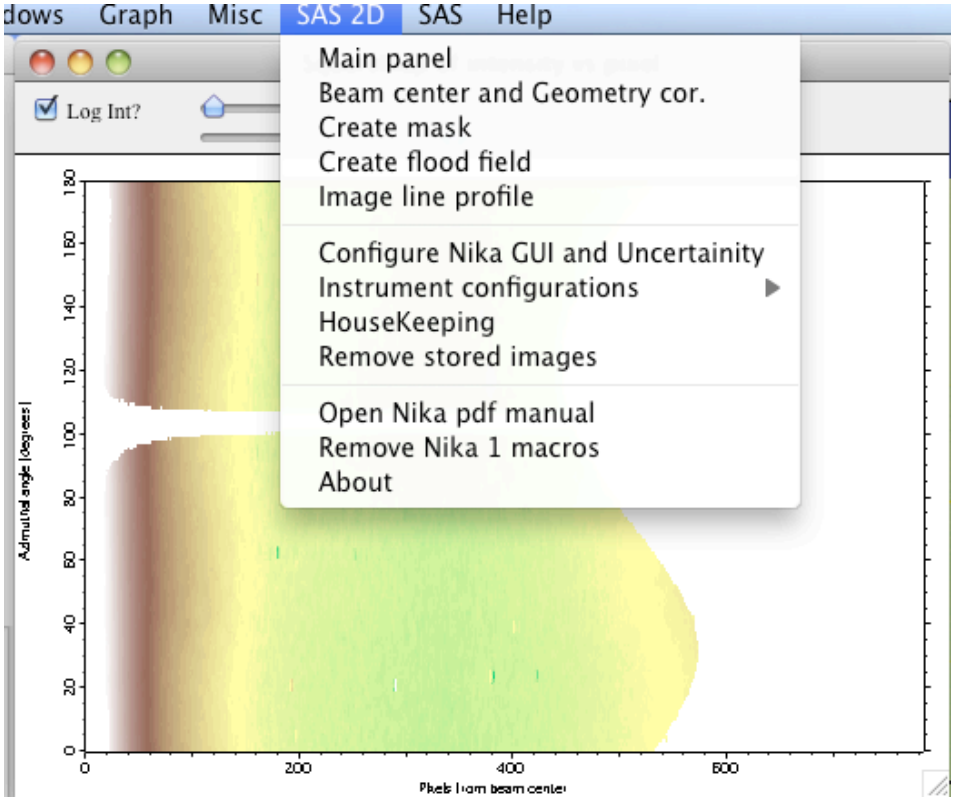
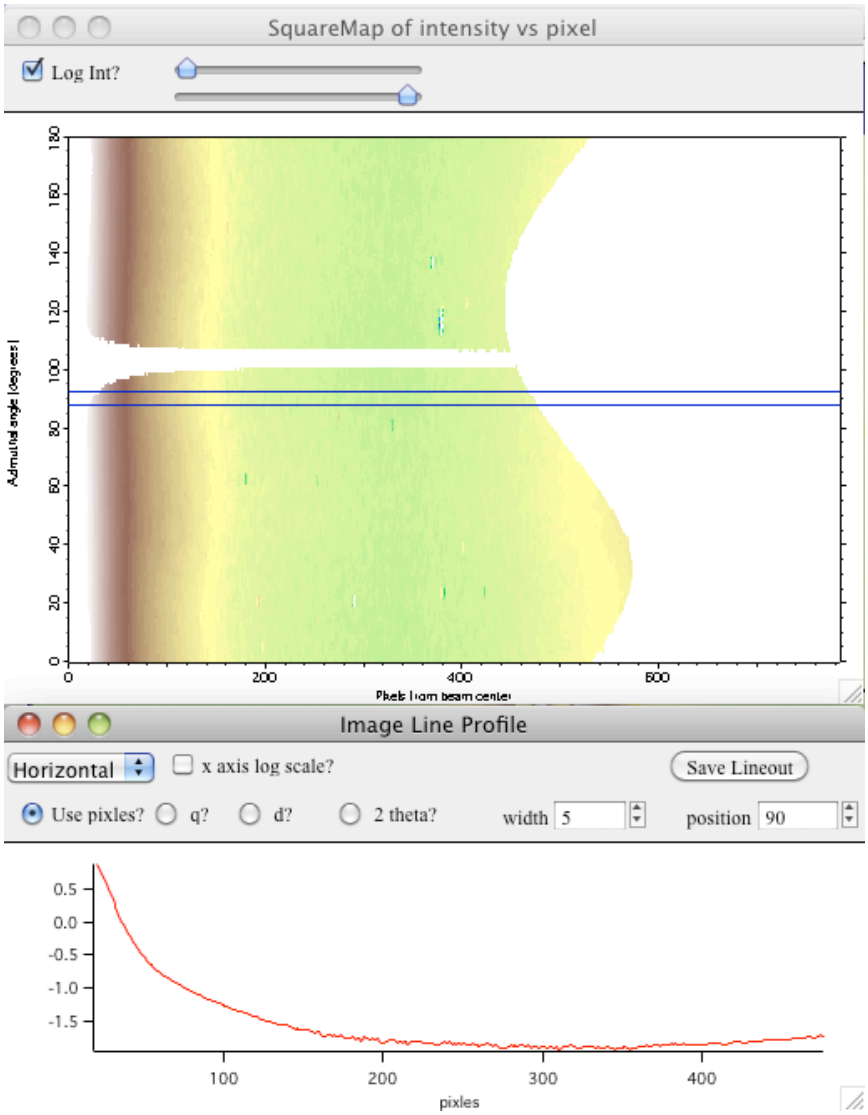
This is plot of radial lineout intensities in sectors (2deg wide in this case). On left axis is azimuthal angle under which the lineout is taken and on bottom axis is pixel value.

This graph can already tell you much easier, if sample is isotropic, for example. If there is diffraction line, if it is strained (line becomes wavy curve) etc.

To be more helpful user can use “lien profile” tool to read more calibrated data from the images. Make sure the image “Square map of intensity vs pixel” is the selected window and from SAS 2D menu select “Image Line profile”:





The new graph now shows the profile of values from the image (in the current setting, it is log-Intensity) vs Pixesl, q, d, or 2 Theta, depending on user choice. X axis can be log or lin… And line can be horizontal or vertical.

Change to Q units, x-axis log-scale:

You can see you can get lineout as needed through various features on the image. You can drag the blue lines in the figure using mouse, change width of the area integrated using "Width" field (in pixels, integers only) and even move position to defined pixel position.

To remove this tool, close first "Image line profile" window and the tool will disappear.

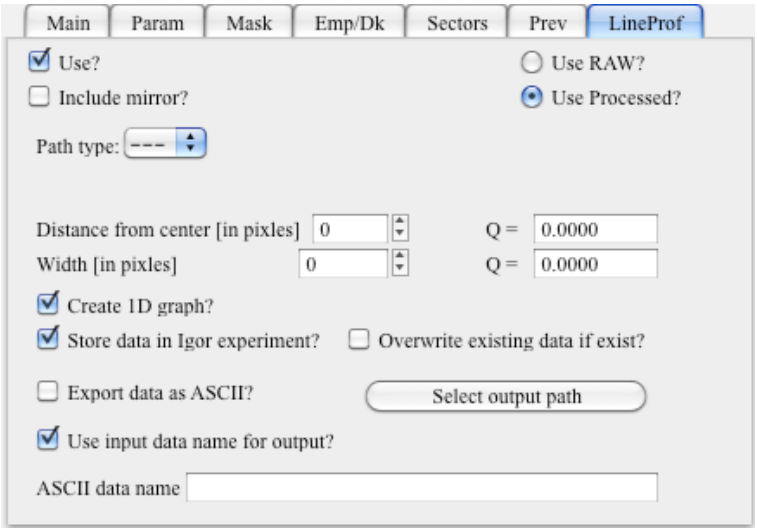
NOTE: Image line profile can be also used on image of the detector itself. But the "Image Line profile" graph will not have some of the capabilities it has on this other window.

LineProf tab

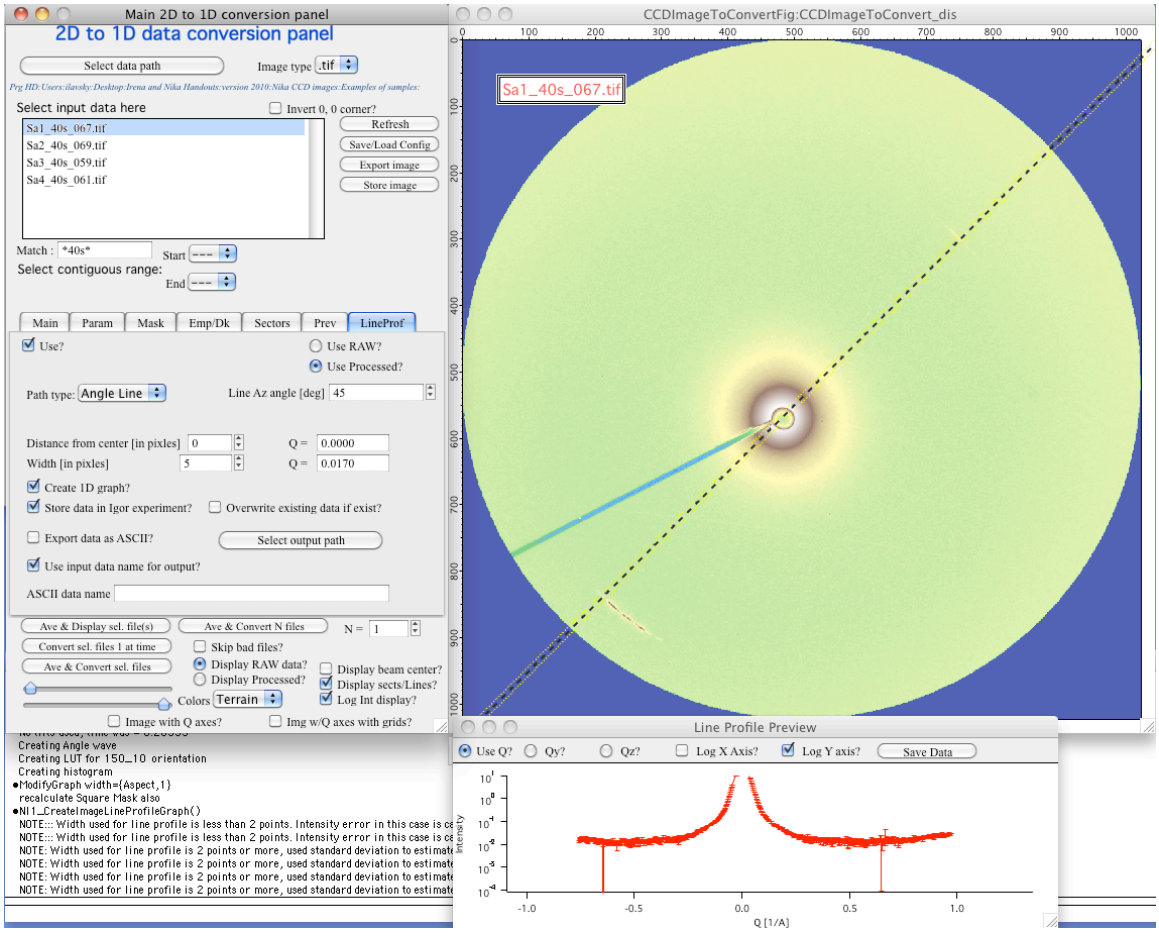
OK, this must be really confusing, but this is different tool that the "Image Line profile" discussed above.

This tool controlled on the last tab enables user to generate Intensity profiles along specific lines/curves on the image. This is also tool, which enables analysis of Grazing incidence geometry, as this seems to be the only really applicable tool…

Select "Use" on the "LineProf" tab:



Let's try to get profile along line at 45 degrees passing though the beam center:



Note, you can control distance from beam center (in pixles), Azimuthal angle, width is pixels etc. You can then create graph, save data or have data automatically processed and saved every time you use one of "Convert …" buttons.

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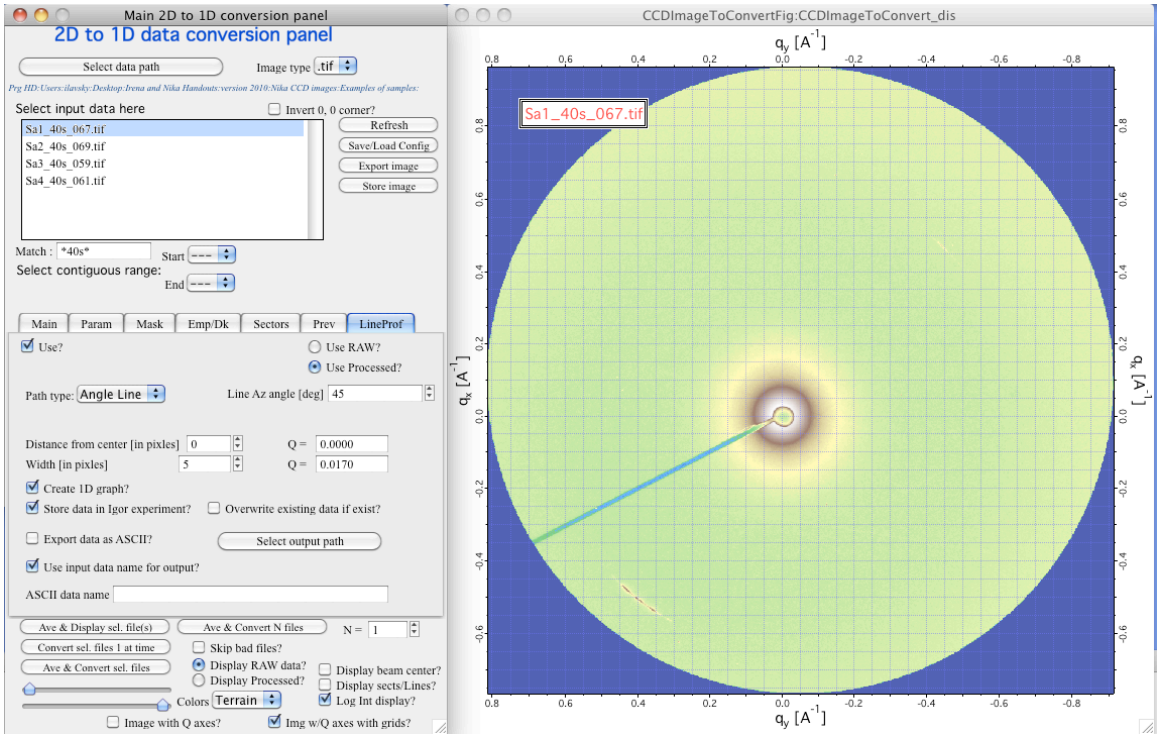
This tool is especially useful for obtaining diffraction peaks along specific direction, analysis of Grazing incidence data (both small-angle scattering and diffraction), or obtaining intensity variation along specific ellipse/circle on the detector.

Some fun stuff

OK, Nika has got lately some fun stuff too. You can display the main image either with pixles on axis – which is not very informative. In case you would like to understand it more, you can change the image axis to Q units. Simply select one of the two checkboxes at the bottom of the Main panel:



You can then actually read directly positions of diffraction peaks from the image… Useful.

Final comment:

Nika can do a lot more than shown here. It can be customized a lot, process multiple data easily and even extended to read ASCII log files to extract transmissions, monitor counts etc. This makes it very useful… BUT, one needs to read included manual. Please, use “Open Nika pdf manaual” command:

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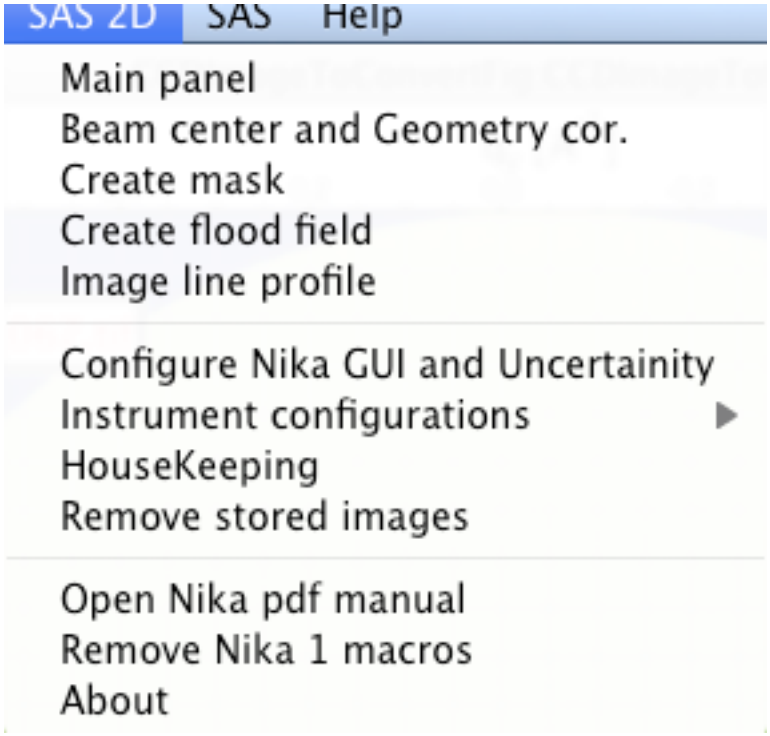

And if everything else fails, send me an e-mail.